## MATERIAL SAFETY DATA SHEET

#### 1. SUBSTANCE AND SOURCE IDENTIFICATION

National Institute of Standards and Technology

**Standard Reference Materials Program** 

100 Bureau Drive, Stop 2320

Gaithersburg, Maryland 20899-2320

SRM Number: 1647e MSDS Number: 1647e

SRM Name: Priority Pollutant Polycyclic Aromatic Hydrocarbons (in Acetonitrile)

Date of Issue: 06 March 2006

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**Description:** Standard Reference Material (SRM) 1647e consists of five 2 mL ampoules, each

containing approximately 1.2 mL of an acetonitrile solution of 16 polycyclic

aromatic hydrocarbons (PAHs).

Substance: Polycyclic Aromatic Hydrocarbons (PAHs) in Acetonitrile

# 2. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS<sup>1</sup>

Component: Acetonitrile

Other Designations: Acetonitrile (cyanomethane; ethanenitrile; ethyl nitrile; methanecarbonitrile;

methyl cyanide)

**CAS Number:** 75-05-8 **EC Number (EINECS):** 200-835-2

**SRM Nominal** 

Concentration (mass %): > 99 EC Classification: F, Xn, Xi

EC Risk (R No.): 11, 20, 21, 22, 36 EC Safety (S No.): 1, 2, 16, 36, 37

#### 3. HAZARDS IDENTIFICATION

**NFPA Ratings (Scale 0–4):** Health = 2 Fire = 3 Reactivity = 0

**Major Health Hazards:** Respiratory tract irritation. Eye irritation. Blood damage.

**Physical Health Hazards:** Flammable liquid and vapor. Vapor may cause flash fire.

**Potential Health Effects** 

**Inhalation:** Inhalation (acute exposure) of acetonitrile with an exposure of 500 ppm for a

short duration may cause irritation of the nose and throat. Exposure to 160 ppm for 4 hours may cause delayed flushing of the face, slight bronchial tightness, a burning sensation, wheezing, and laryngitis. High concentration exposure may cause delayed coughing, bloody sputum, nausea, chest pain, headache, dizziness, low blood pressure, rapid pulse, respiratory depression, weakness, confusion, convulsions, unconsciousness, coma, and death due to central nervous system

depression.

Skin Contact: Skin contact with acetonitrile may cause irritation. Skin absorption may occur

and result in systemic toxicity with symptoms similar to acute inhalation.

Repeated or prolonged exposure may cause dermatitis.

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<sup>&</sup>lt;sup>1</sup> Hazardous components 1 % or greater; Carcinogens 0.1 % or greater are listed in compliance with OSHA 29 CFR 1910.1200. For the list and actual concentration of hazardous PAHs less than 1 %, and carcinogen PAHs less than 0.1 % which are below the reportable limit, refer to the corresponding Certificate of Analysis.

**Eye Contact:** Eye contact with acetonitrile liquid and vapors may cause irritation and tearing.

Repeated or prolonged exposure may cause conjunctivitis.

**Ingestion:** Ingestion may cause systemic toxicity as described in acute inhalation.

Listed as a Carcinogen/ Potential Carcinogen:

Acetonitrile

Yes No X

In the National Toxicology Program (NTP) Report on Carcinogens.

In the International Agency for Research on Cancer (IARC)

Monographs.

By the Occupational Safety and Health Administration (OSHA).

4. FIRST AID MEASURES

Inhalation: If adverse effects occur, remove to uncontaminated area. Give artificial

respiration, if not breathing, by qualified personnel. Get immediate medical

attention.

**Skin Contact:** Rinse affected area with copious amounts of water for at least 15 minutes while

removing contaminated clothing. Get medical attention, if needed.

Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of

water for at least 15 minutes. Get immediate medical attention.

**Ingestion:** Get immediate medical attention. **DO NOT** induce vomiting. If vomiting

occurs, keep head lower than hips to prevent aspiration. Give artificial

respiration, if not breathing, by qualified personnel.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards: Acetonitrile is a severe fire hazard. Vapors, which are heavier that air, may

ignite from distant ignition sources. Flash backs may occur.

**Extinguishing Media:** Regular dry chemical. Carbon dioxide. Water. Alcohol resistant foam.

**Fire Fighting:** Move container from fire area if it can be done without risk. Use water spray to

cool containers until well after the fire is out and to discharge vapors. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus

(SCBA).

Acetonitrile

**Flash Point:** 6 °C (43 °F) **Method Used:** Open cup.

**Autoignition Temp.:** 524 °C (975 °F)

Flammability Class (OSHA): IB

Flammability Limits in Air

UPPER (Volume %): 16
LOWER (Volume %): 3

6. ACCIDENTAL RELEASE MEASURES

Occupational Release: Avoid heat, flames, sparks, and other sources of ignition. Reduce vapors with

water spray. Collect small spilled material after absorbing with sand or other non-combustible material in an appropriate container for disposal. For large spills, stop leak if possible without personal risk. Notify Local Emergency Planning Committee and State Emergency Response Commission for release greater than or equal to the Release Quantity (RQ) (see Section 15, "Regulatory

Information"). Keep out of water supplies and sewers.

Reportable Quantity (RQ): Acetonitrile is subject to RQ under Title III of SARA, which is greater than the

unit quantity provided for SRM 1647e. See Section 15, "Regulatory

Information".

**Disposal:** Refer to Section 13, "Disposal Considerations".

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### 7. HANDLING AND STORAGE

Storage: Store and handle in accordance with all current regulations and standards. Store

with flammable liquids. Keep separated from incompatible substances. Refer to

SRM 1647e Certificate of Analysis for storage of SRM 1647e.

**Safe Handling Precautions:** See Section 8, "Exposure Controls and Personal Protection".

#### 8. EXPOSURE CONTROLS AND PERSONAL PROTECTION

**Exposure Limits:** Acetonitrile

OSHA (PEL): 70 mg/m<sup>3</sup> (40 ppm) TWA

ACGIH: 20 ppm TWA (skin)

NIOSH: 34 mg/m<sup>3</sup> (20 ppm) recommended TWA (10 h)

UK WEL: 68 mg/m<sup>3</sup> (40 ppm) TWA UK WEL: 102 mg/m<sup>3</sup> (60 ppm) STEL

Ventilation: Use local exhaust ventilation system. Ventilation equipment should be

explosion-resistant if explosive concentrations of material are present. Ensure

compliance with applicable exposure limits.

**Respirator:** If necessary, refer to the "NIOSH Guide to the Selection and Use of Particulate

Respirators Certified under 42 CFR 84" for selection and use of respirators with

organic vapor cartridges certified by NIOSH.

**Eye Protection:** Wear safety goggles. An eye wash station should be readily available near areas

of use.

**Personal Protection:** Wear appropriate protective clothing and chemically resistant gloves to prevent

skin exposure.

#### 9. PHYSICAL AND CHEMICAL PROPERTIES

**Component:** Acetonitrile

**Appearance and Odor:** Liquid. Colorless. Sweet odor.

Relative Molecular Mass: 41.05 Molecular Formula: CH<sub>3</sub>CN

**Boiling Point:** 82 °C (180 °F) **Freezing Point:** -46 °C (-51 °F) **Density (23 °C):** 0.7789 g/cm<sup>3</sup> **Water Solubility:** Soluble.

Solvent Solubility: Soluble in alcohol, ether, acetone, benzene, methyl acetate, ethyl acetate,

chloroform, carbon tetrachloride, ethylene chloride, acetamide solutions, and

unsaturated hydrocarbons.

**Odor Threshold:** 40 ppm

#### 10. STABILITY AND REACTIVITY

Stability: X Stable Unstable

Stable at normal temperatures and pressure.

Conditions to Avoid: Avoid heat, flames, sparks, and other sources of ignition. Containers may

rupture or explode if exposed to heat. Keep out of water supplies and sewers.

Avoid contact and inhalation of material or combustion by-products.

**Incompatible Materials:** Acids. Metals. Bases. Oxidizing materials. Combustible materials. Reducing

agents.

**Fire/Explosion Information:** See Section 5, "Fire Fighting Measures".

**Hazardous Decomposition:** Thermal decomposition can produce oxides of carbon, nitrogen oxides, and

cvanide fumes.

Hazardous Polymerization: Will Occur X Will Not Occur

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## 11. TOXICOLOGICAL INFORMATION

Route of Entry: X Inhalation X Skin X Ingestion

**Toxicity Data:** Acetonitrile

Man, Oral TD<sub>LO</sub>: 64 mg/kg Woman, Oral TD<sub>LO</sub>: 500 mg/kg Human, Inhalation TC<sub>LO</sub>: 160 ppm (4 h)

Rat, Oral LD<sub>50</sub>: 2 460 mg/kg

Tumorigenic, Reproductive,

Mutagenic Data: Acetonitrile has been investigated as a tumorigenic, reproductive, and mutagenic

effector.

**Health Effects** 

(Acute and Chronic): See Section 3, "Hazards Identification" for potential health effects.

12. ECOLOGICAL INFORMATION

**Ecotoxicity Data:** Highly toxic to aquatic life.

13. DISPOSAL CONSIDERATIONS

**Waste Disposal:** Dispose in accordance with all applicable federal, state, and local regulations.

Acetonitrile is subject to disposal regulations, U.S. EPA 40 CFR 262, Hazardous

Waste Number U003.

14. Transportation Information

**U.S. DOTand IATA:** Acetonitrile; Excepted Quantity (1.2 mL × 5), UN1648; Hazard Class 3;

Packing Group II.

15. REGULATORY INFORMATION

U.S. Regulations: CERCLA Sections 102a/103 (40 CFR 302.4): Acetonitrile: 2 272.7 kg

(5 000 lbs) RQ.

SARA Title III Section 302 (40 CFR 355.30): Not regulated. SARA Title III Section 304 (40 CFR 355.40): Not regulated. SARA Title III Section 313 (40 CFR 372.65): Acetonitrile. OSHA Process Safety (29 CFR 1910.119): Not regulated.

SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21):

ACUTE: Yes.
CHRONIC: No.
FIRE: Yes.
REACTIVE: No.

SUDDEN RELEASE: No.

**State Regulations:** California Proposition 65: Not regulated.

**CANADIAN Regulations** 

WHMIS Classification: Not determined.

**EUROPEAN Regulations** 

**EC Classification (assigned):** F Highly Flammable.

Xn Harmful. Xi Irritant.

**EC Risk Phrases:** R 11 Highly flammable.

R 20/21/22 Harmful by inhalation, in contact with skin, and if swallowed.

R 36 Irritating to eyes.

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**EC Safety Phrases:** S 1/2 Keep locked up and out of reach of children.

S 16 Keep away from sources of ignition.

S 36/37 Wear suitable protective clothing and gloves.

**National Inventory Status** 

**U.S. Inventory (TSCA):** Acetonitrile: Listed on inventory.

**TSCA 12(b)** 

**Export Notification:** Acetonitrile: CAS No: 75-05-8

Section 4

## 16. OTHER INFORMATION

**Sources:** MDL Information Systems, Inc., MSDS *Acetonitrile*, 15 September 2005.

**Disclaimer:** Physical and chemical data contained in this MSDS are provided only for use as a guide in assessing the hazardous nature of the material. The MSDS was prepared carefully, using current references; however, NIST does not certify the data in the MSDS. The certified values for this material are given in the NIST Certificate of Analysis.

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